

# Two-Qubit Separability Probabilities and Beta Functions

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(Dated: February 1, 2008)

## Abstract

Due to recent important work of Życzkowski and Sommers (*J. Phys. A* **36**, 10115 [2003] and **36**, 10083 [2003]), exact formulas are available (both in terms of the Hilbert-Schmidt and Bures metrics) for the  $(n^2 - 1)$ -dimensional and  $(\frac{n(n-1)}{2} - 1)$ -dimensional volumes of the complex and real  $n \times n$  density matrices. However, no comparable formulas are available for the volumes (and, hence, probabilities) of various separable subsets of them. We seek to clarify this situation for the Hilbert-Schmidt metric for the simplest possible case of  $n = 4$ , that is, the two-qubit systems. Making use of the density matrix ( $\rho$ ) parameterization of Bloore (*J. Phys. A* **9**, 2059 [1976]), we are able to reduce each of the real and complex volume problems to the calculation of a *one*-dimensional integral, the single relevant variable being a certain ratio of diagonal entries,  $\nu = \frac{\rho_{11}\rho_{44}}{\rho_{22}\rho_{33}}$ . The associated integrand in each case is the product of a *known* (highly oscillatory near  $\nu = 1$ ) jacobian and a certain *unknown* univariate function, which our extensive numerical (quasi-Monte Carlo) computations indicate is very closely proportional to an (incomplete) beta function  $B_\nu(a, b)$ , with  $a = \frac{1}{2}, b = \sqrt{3}$  in the real case, and  $a = \frac{2\sqrt{6}}{5}, b = \frac{3}{\sqrt{2}}$  in the complex case. Assuming the full applicability of these specific incomplete beta functions, we undertake separable volume calculations.

**Mathematics Subject Classification (2000):** 81P05, 52A38, 15A90, 81P15

PACS numbers: Valid PACS 03.67.-a, 02.30.Gp, 02.40.Dr, 02.40.Ft, 02.60.-x

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## I. INTRODUCTION

In a pair of major, skillful papers, making use of the theory of random matrices [1], Sommers and Życzkowski were able to derive explicit formulas for the volumes occupied by the  $d = (n^2 - 1)$ -dimensional convex set of  $n \times n$  (complex) density matrices (as well as the  $d = \frac{(n-1)(n+2)}{2}$ -dimensional convex set of real (symmetric)  $n \times n$  density matrices), both in terms of the Hilbert-Schmidt (HS) metric [2] — inducing the flat, Euclidean geometry — and the Bures metric [3] (cf. [4]). Of course, it would be of obvious considerable quantum-information-theoretic interest in the cases that  $n$  is a composite number, to also obtain HS and Bures volume formulas restricted to those states that are separable — the sum of product states — in terms of some factorization of  $n$  [5]. Then, by taking ratios — employing these Sommers-Życzkowski results — one would obtain corresponding separability *probabilities*. (In an *asymptotic* regime, in which the dimension of the state space grows to infinity, Aubrun and Szarek recently concluded [6] that for qubits and larger-dimensional particles, the proportion of the states that are separable is superexponentially small in the dimension of the set.)

In particular, again for the 15-dimensional complex case,  $n = 4 = 2 \times 2$ , numerical evidence has been adduced that the Bures volume of separable states is (quite elegantly)  $2^{-15}(\frac{\sqrt{2}-1}{3}) \approx 4.2136 \cdot 10^{-6}$  [7, Table VI] and the HS volume  $(5\sqrt{3})^{-7} \approx 2.73707 \cdot 10^{-7}$  [8, eq. (41)]. Then, taking ratios (using the corresponding Sommers-Życzkowski results), we have the derived conjectures that the Bures separability probability is  $\frac{1680(\sqrt{2}-1)}{\pi^8} \approx 0.0733389$  and the HS one, considerably larger,  $\frac{2^2 \cdot 3 \cdot 7^2 \cdot 11 \cdot 13 \sqrt{3}}{5^4 \pi^6} \approx 0.242379$  [8, eq. (43), but misprinted as  $5^3$  not  $5^4$  there]. (Szarek, Bengtsson and Życzkowski — motivated by the numerical findings of [8, 9] — have recently formally demonstrated “that the probability to find a random state to be separable equals 2 times the probability to find a random boundary state to be separable, provided the random states are generated uniformly with respect to the Hilbert-Schmidt (Euclidean) distance. An analogous property holds for the set of positive-partial-transpose states for an arbitrary bipartite system” [10] (cf. [11]). These authors also noted [10, p. L125] that “one could try to obtain similar results for a general class of multipartite systems”. In this latter vein, preliminary numerical analyses of ours have given some [but certainly not yet conclusive] indication that for the *three-qubit triseparable* states, there may be an analogous probability ratio of 6 — rather than 2.)

However, the analytical derivation of (conjecturally) exact formulas for these HS and Bures (as well as other, such as the Kubo-Mori [12] and Wigner-Yanase [8, 13]) separable volumes has seemed quite remote — the only analytic progress to report so far being certain exact formulas when the number of dimensions of the 15-dimensional space of  $4 \times 4$  density matrices has been severely curtailed (nullifying or holding constant *most* of the 15 parameters) to  $d \leq 3$  [14, 15] (cf. [16]). Most strikingly, in this research direction, in [15, Fig. 11], we were able to find a highly interesting/intricate (one-dimensional) continuum ( $-\infty < \beta < \infty$ ) of two-dimensional (the associated parameters being  $b_1$ , the mean, and  $\sigma_q^2$ , the variance of the Bell-CHSH observable) HS separability probabilities, in which the *golden ratio* [17] was featured — serving to demarcate different separability regimes — among other items. (The associated HS volume element —  $\frac{1}{32\beta(1+\beta)}d\beta db_q d\sigma_q^2$  — is independent of  $b_1$  and  $\sigma_q^2$  in this three-dimensional scenario.) Further, in [14], building upon work of Jakóbczyk and Siennicki [18], we obtained a remarkably wide-ranging variety of exact HS separability ( $n = 4, 6$ ) and PPT (positive partial transpose) ( $n = 8, 9, 10$ ) probabilities based on *two*-dimensional sections of sets of (generalized) Bloch vectors corresponding to  $n \times n$  density matrices.

Nevertheless, computations for the *full*  $d = 9$  and/or  $d = 15$ ,  $n = 4$  real and complex two-qubit scenarios are quite daunting — due to the numerous separability constraints at work, some being active [binding] in certain regions and in complementary regions, inactive [nonbinding]. “The geometry of the 15-dimensional set of separable states of two qubits is not easy to describe” [10, p. L125]. We seek to make substantial progress in these directions here, and, in fact, prove able to recast both these problems within *one*-dimensional frameworks.

We accomplish this dimensional reduction through the use of the (quite simple) form of parameterization of the density matrices put forth by Bloore [19, 20] some thirty years ago. (Of course, there are a number of other possible parametrizations [21, 22, 23, 24, 25, 26, 27], several of which we have also utilized in various studies [28, 29] to estimate volumes of separable states. Our greatest progress at this stage, in terms of increasing dimensionality, though, has been achieved with the Bloore parameterization — due to a certain computationally attractive feature of it, allowing one to *decouple* diagonal and non-diagonal parameters — which is described in sec. II.)

### A. Outline of paper

In sec. II immediately below, we describe the Bloore density matrix parameterization. Then, we present in sec. III the specific one-dimensional integration formulas we have obtained for the real and complex HS separable qubit-qubit volumes using the Bloore parameterization. The integrands in each of these cases are the product of a *known* jacobian function and a heretofore *uncharacterized* function. In sec. IV, we detail the extensive numerical (quasi-Monte Carlo) procedures employed to estimate these unknown functions. Then, in sec. V, we demonstrate — quite unanticipatedly — that our estimates of these functions over the unit interval are remarkably well-fitted (up to proportionality constants) by certain specific incomplete beta functions. In the complex case, we can perform the indicated separable-volume integration exactly, but only numerically in the real case. In sec. VI, we give some concluding remarks.

In any case, it appears that further research is called for, to formally establish or appropriately qualify the role of the incomplete beta function in the determination of the real and complex two-qubit Hilbert-Schmidt *separable* volumes.

## II. BLOORE PARAMETERIZATION OF DENSITY MATRICES

The main presentation of Bloore [19] was made in terms of the  $3 \times 3$  ( $n = 3$ ) density matrices. It is clearly easily extendible to cases  $n > 3$ . The fundamental idea is to scale the off-diagonal elements ( $\rho_{ij}, i \neq j$ ) of the density matrix in terms of the square roots of the diagonal entries ( $\rho_{ii}$ ). That is, one sets (introducing the new [Bloore] variables  $z_{ij}$ ),

$$\rho_{ij} = \sqrt{\rho_{ii}\rho_{jj}}z_{ij}. \quad (1)$$

This allows the determinant of  $\rho$  (and analogously all its principal minors) to be expressible as the *product* ( $|\rho| = A_1 A_2$ ) of two factors, one ( $A_1 = \prod_{i=1}^4 \rho_{ii}$ ) of which is itself simply the product of (nonnegative) diagonal entries ( $\rho_{ii}$ ). In the real  $n = 4$  case under investigation here — we have

$$A_2 = (z_{34}^2 - 1)z_{12}^2 + 2(z_{14}(z_{24} - z_{23}z_{34}) + z_{13}(z_{23} - z_{24}z_{34}))z_{12} - z_{23}^2 - z_{24}^2 - z_{34}^2 + \quad (2)$$

$$z_{14}^2(z_{23}^2 - 1) + z_{13}^2(z_{24}^2 - 1) + 2z_{23}z_{24}z_{34} + 2z_{13}z_{14}(z_{34} - z_{23}z_{24}) + 1,$$

involving (only) the  $z_{ij}$ 's ( $i > j$ ), where  $z_{ji} = z_{ij}$  [19, eqs. (15), (17)]. Since, clearly, the factor  $A_1$  is positive in all nondegenerate cases ( $\rho_{ii} > 0$ ), one can — by only analyzing  $A_2$  — essentially ignore the diagonal entries, and thus reduce by  $(n - 1)$  the dimensionality of the problem of finding nonnegativity conditions to impose on  $\rho$ . This is the feature we have sought to maximally exploit above. A fully analogous decoupling property holds in the complex case.

It is, of course, necessary and sufficient for  $\rho$  to serve as a density matrix (that is, an Hermitian, nonnegative definite, trace one matrix) that all its principal minors be nonnegative [30]. The (necessary — but not sufficient) condition — quite natural in the Bloore parameterization — that all the principal  $2 \times 2$  minors be nonnegative requires simply that  $-1 \leq z_{ij} \leq 1, i \neq j$ . The joint conditions that *all* the principal minors be nonnegative are not as readily apparent. But for the 9-dimensional *real* case  $n = 4$  — that is,  $\Im(\rho_{ij}) = 0$  — we have been able to obtain one such set, using the Mathematica implementation of the *cylindrical algorithm decomposition* (CAD) [31]. (The set of solutions of any system of real algebraic equations and inequalities can be decomposed into a finite number of “cylindrical” parts [32].) Applying it, we were able to express the conditions that an arbitrary 9-dimensional  $4 \times 4$  real density matrix  $\rho$  must fulfill. These took the form,

$$z_{12}, z_{13}, z_{14} \in [-1, 1], z_{23} \in [Z_{23}^-, Z_{23}^+], z_{24} \in [Z_{24}^-, Z_{24}^+], z_{34} \in [Z_{34}^-, Z_{34}^+], \quad (3)$$

where

$$\begin{aligned} Z_{23}^\pm &= z_{12}z_{13} \pm \sqrt{1 - z_{12}^2}\sqrt{1 - z_{13}^2}, Z_{24}^\pm = z_{12}z_{14} \pm \sqrt{1 - z_{12}^2}\sqrt{1 - z_{14}^2}, \\ Z_{34}^\pm &= \frac{z_{13}z_{14} - z_{12}z_{14}z_{23} - z_{12}z_{13}z_{24} + z_{23}z_{24} \pm s}{1 - z_{12}^2}, \end{aligned} \quad (4)$$

and

$$s = \sqrt{-1 + z_{12}^2 + z_{13}^2 - 2z_{12}z_{13}z_{23} + z_{23}^2}\sqrt{-1 + z_{12}^2 + z_{14}^2 - 2z_{12}z_{14}z_{24} + z_{24}^2}. \quad (5)$$

Making use of these results, we were able to confirm *via* exact symbolic integrations, the (formally demonstrated) result of Życzkowski and Sommers [2] that the HS volume of the *real* two-qubit ( $n = 4$ ) states is  $\frac{\pi^4}{60480} \approx 0.0016106$ . (We could also verify this through a somewhat [superficially, at least] different Mathematica computation, using the implicit integration feature first introduced in version 5.1. That is, the only integration limits employed were that  $z_{ij} \in [-1, 1], i \neq j$  — *broader* than those yielded by the CAD given by (3) — while the Boolean constraints were now imposed that the determinant of  $\rho$  and *one* [all that is needed to ensure nonnegativity] of its principal  $3 \times 3$  minors be nonnegative.)

## A. Determinant of the Partial Transpose

However, when we tried to combine these CAD integration limits (3) with the (Peres-Horodecki [33, 34, 35]  $n = 4$ ) separability constraint that the determinant ( $A_3 = |\rho_{PT}|$ ) of the partial transpose of  $\rho$  be nonnegative [36, Thm. 5], we exceeded the memory availabilities of our workstations. In general, the term  $A_3$  — unlike the earlier term  $A_2$  — unavoidably involves the diagonal entries ( $\rho_{ii}$ ), so the dimension of the accompanying integration problems must increase, it would seem, we initially thought — in the 9-dimensional real  $n = 4$  case from six to nine.

### 1. Role of univariate ratio of diagonal entries

However, we then noted that, in fact, the dimensionality of the required integrations for the separable volumes must only essentially be increased by one (rather than three) from that for the total volumes, since  $A_3$  turns out to be (aside from the necessarily nonnegative factor of  $A_1$ , which we can ignore) expressible solely in terms of the (six, in the real case) distinct  $z_{ij}$ 's and the (*univariate*) ratio

$$\nu = \frac{\rho_{11}\rho_{44}}{\rho_{22}\rho_{33}}. \quad (6)$$

(Numerical probes of ours demonstrated that  $\nu$  is *not* a local invariant of two-qubit mixed states, in the sense of Makhlin [37].) We, then, have

$$A_3 \equiv |\rho_{PT}| = A_1 \left( -z_{14}^2\nu^2 + 2z_{14}(z_{12}z_{13} + z_{24}z_{34})\nu^{3/2} + s\nu + 2z_{23}(z_{12}z_{24} + z_{13}z_{34})\nu^{1/2} - z_{23}^2 \right), \quad (7)$$

where

$$s = (z_{34}^2 - 1)z_{12}^2 - 2(z_{14}z_{23} + z_{13}z_{24})z_{34}z_{12} - z_{13}^2 + z_{14}^2z_{23}^2 + (z_{13}^2 - 1)z_{24}^2 - z_{34}^2 - 2z_{13}z_{14}z_{23}z_{24} + 1.$$

$A_3$  is, thus, a *quartic/biquadratic* polynomial in terms of  $\sqrt{\nu}$  (cf. [23, 38]). (Clearly, the difficulty of the two-qubit separable-volume problem under study here is strongly tied to the high [fourth] degree of  $A_3$  in  $\sqrt{\nu}$ . By setting either  $z_{14} = 0$  or  $z_{23} = 0$ , the degree of  $A_3$  can be reduced to 2 (cf. [20]).) In the *complex* case,  $A_{3_{\text{complex}}}$  — which we do not explicitly present here — also assumes the form of a quartic polynomial in  $\sqrt{\nu}$ . So one must deal, in such a setting, with 13-dimensional integration problems rather than 15-dimensional ones.

## 2. attempted seven-fold exact integration

The problem of determining the separable volumes can, thus, be seen to hinge on (in the real case), a *seven*-fold integration involving the six (independent)  $z_{ij}$ 's and  $\nu$ . However, such requisite integrations, allowing  $\nu$  to vary (or even holding  $\nu$  constant at various values, such as  $\nu = 1$ , thus, reducing to six-fold integrations), did not appear — rather frustratingly, we must admit — to be exactly/symbolically performable (using version 5.2 of Mathematica).

### III. REDUCTION TO ONE-DIMENSIONAL PROBLEMS

Making use of the “Bloore parameterization” [19] (sec. II immediately above) of density matrices, which allows the decoupling of diagonal entries from non-diagonal entries in certain relevant determinant calculations, one can show that the problem of computing the 15-dimensional volume ( $V_{sep/complex}$ ) of the *separable* two-qubit systems is reducible to a *one*-dimensional integration of the form,

$$V_{sep/complex} = 2 \int_0^1 Jac_{complex}(\nu) F_{complex}(\nu) d\nu. \quad (8)$$

(We measure volume in terms of the Euclidean/Hilbert-Schmidt/Frobenius norm, and slightly modify our notation in [39], to indicate that we have changed from the variable  $\mu$  used there to  $\nu \equiv \mu^2$  here. The variable  $\nu$  — as noted earlier (6) — is simply a specific ratio  $\frac{\rho_{11}\rho_{44}}{\rho_{22}\rho_{33}}$  of diagonal entries  $\rho_{ii}$  of the corresponding  $4 \times 4$  density matrices  $\rho$ .)

Similarly, the 9-dimensional Hilbert-Schmidt volume of the separable real density matrices (those with entries restricted to the real numbers) can be expressed as

$$V_{sep/real} = 2 \int_0^1 Jac_{real}(\nu) F_{real}(\nu) d\nu. \quad (9)$$

The two (highly oscillatory near  $\nu = 1$ ) jacobian functions ( $Jac_{real}(\nu)$  and  $Jac_{complex}(\nu)$ ) are both explicitly known [39, sec. III.B], that is (Fig. 1),

$$Jac_{real}(\nu) = \frac{\nu^{3/2} (12 (\nu(\nu + 2) (\nu^2 + 14\nu + 8) + 1) \log(\sqrt{\nu}) - 5 (5\nu^4 + 32\nu^3 - 32\nu - 5))}{3780(\nu - 1)^9} \quad (10)$$

and (Fig. 2)

$$Jac_{complex}(\nu) = -\frac{\nu^3}{3603600(\nu - 1)^{15}} (h_1 + h_2), \quad (11)$$

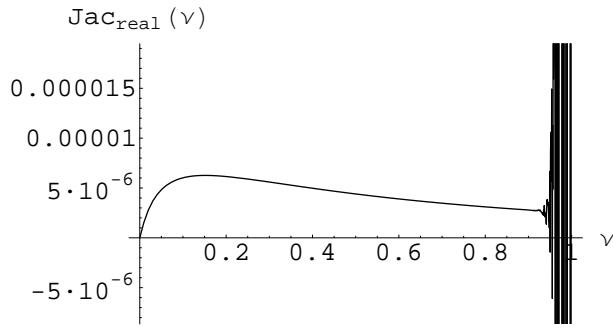


FIG. 1: Plot of the jacobian function  $Jac_{real}(\nu)$ , given by (10)

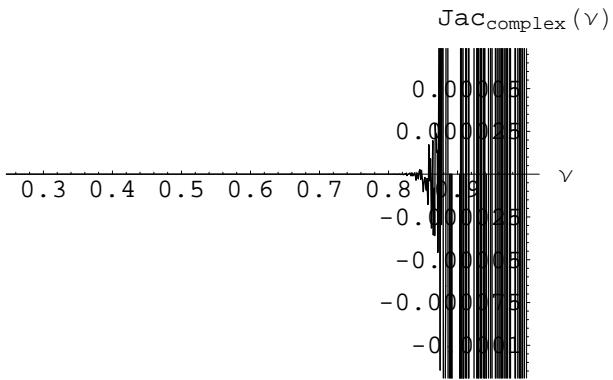


FIG. 2: Plot of the jacobian function  $Jac_{complex}(\nu)$ , given by (11)

where

$$h_1 = 363\nu^7 + 9947\nu^6 + 48363\nu^5 + 42875\nu^4 - 42875\nu^3 - 48363\nu^2 - 9947\nu - 363;$$

$$h_2 = -140 (\nu^7 + 49\nu^6 + 441\nu^5 + 1225\nu^4 + 1225\nu^3 + 441\nu^2 + 49\nu + 1) \log(\sqrt{\nu}).$$

We obtained the jacobian functions  $Jac_{real}(\nu)$  and  $Jac_{complex}(\nu)$ , given in (10) and (11), by transformations of, say,  $\rho_{33}$  to the  $\nu$  variable (and subsequent two-fold exact integrations over  $\rho_{11}$  and  $\rho_{22}$ ) of the original (three-dimensional) jacobians, involving the diagonal entries, for the Bloore parameterizations. These original jacobians were of the form  $(\prod_{i=1}^4 \rho_{ii})^k$  with  $k = \frac{3}{2}$  in the real case, and  $k = 3$ , in the complex case. (Of course, by the unit trace condition, we must have  $\rho_{44} = 1 - \rho_{11} - \rho_{22} - \rho_{33}$ .)

The (only) unknowns in our two separable-volume-computation problems ((8) and (9)) are, then, the functions  $F_{real}(\nu)$  and  $F_{complex}(\nu)$ . In our preprint [39], we reported our

initial numerical (quasi-Monte Carlo) procedures to estimate these two centrally important functions (but in terms of the variable  $\mu = \sqrt{\nu}$ ). We have since continued these efforts, which we now detail in the following section.

#### IV. ESTIMATION OF UNKNOWN UNIVARIATE FUNCTIONS

At an advanced stage of our numerical analyses, the initial results of which had been reported in [39], it appeared that it might be more efficacious to employ  $\nu = \frac{\rho_{11}\rho_{44}}{\rho_{22}\rho_{33}}$  as the principal variable rather than  $\mu = \sqrt{\frac{\rho_{11}\rho_{44}}{\rho_{22}\rho_{33}}}$ . (Thus, as previously noted, we have  $\nu \equiv \mu^2$ .) So, our estimation (*uniform* sampling) procedures were originally designed in terms of  $\mu$ , rather than  $\nu$ .

We had, in [39], begun proceeding along two fully parallel courses, one for the 9-dimensional real two-qubit case and the other for the 15-dimensional complex case. We sought those functions  $f_{real}(\mu)$  and  $f_{complex}(\mu)$ , that we now see satisfy the equivalences,

$$f_{real}(\sqrt{\nu}) \equiv F_{real}(\nu), \quad f_{complex}(\sqrt{\nu}) \equiv F_{complex}(\nu), \quad (12)$$

that would result from imposing the conditions that the expressions  $A_1$ ,  $A_2$  and  $A_3$  (as well as a principal  $3 \times 3$  minor of  $\rho$ ), along with their complex counterpart expressions, be *simultaneously* nonnegative. (The satisfaction of all these joint conditions ensures that we are dealing precisely with *separable*  $4 \times 4$  density matrices.) It was evident that the relation  $f(\mu) = f(\frac{1}{\mu})$  must hold, so we only numerically studied the range  $\mu \in [0, 1]$ . Dividing this unit interval into 2,000 equal nonoverlapping subintervals of length  $\frac{1}{2000}$  each, we sought to estimate the  $f(\mu)$ 's at the 2,001 end points of these subintervals.

This required ( $\mu$  being alternately fixed at every single one of these end points for each set of  $z_{ij}$ 's) numerical integrations in 6 and 12 dimensions. For this purpose, we utilized the Tezuka-Faure (TF) quasi-Monte Carlo procedure [40, 41], we have extensively used in our earlier studies of separability probabilities [7, 8] (cf. [42] for an apparently more efficient approach to estimating the Euclidean volume of *convex* bodies). For each of the 2,001 discrete, equally-spaced values of  $\mu$  we employed the same set of 611,500,000 Tezuka-Faure six-dimensional points in the real case and, similarly, the same set of 549,500,000 twelve-dimensional points in the complex case. (The Tezuka-Faure points are defined over unit hypercubes  $[0, 1]^n$ , so in our computations, we transform the Bloore variables accordingly

and take into account the corresponding jacobians.)

### A. Close comparison with Życzkowski-Sommers known values

In the real case, our sample estimate of the *known* Hilbert-Schmidt volume of (separable *plus* nonseparable) states [2],  $\frac{\pi^4}{60480} \approx 0.0016106$  was smaller by only a factor of 0.999996. So, we would expect our companion estimates of  $f_{real}(\mu)$ , at each of the 2,001 sampled points, to be roughly equally precise. (Let us note that  $f_{real}(0) = f_{complex}(0) = 0$ . Statistical testing — the use of confidence limits — is not appropriate in the Tezuka-Faure framework (cf. [43]).) In the complex case, our estimate of the known 15-dimensional volume,  $\frac{\pi^6}{851350500} \approx 1.12925 \cdot 10^{-6}$  was larger only by a factor of 1.00009.

As instances of specific values (avoiding the necessity for 2,000 repetitions for each point), based on independent analyses using still larger numbers of TF-points, we obtained estimates of  $f_{real}(1) = F_{real}(1) = \frac{1610102144}{14046875} \approx 114.62351$ ,  $f_{real}(\frac{1}{2}) = \frac{1040958844}{14046875} \approx 74.10608$ , both based on 3,596,000,000 TF-points, and  $f_{complex}(1) = F_{complex}(1) = 387.5080921$  and  $f_{complex}(\frac{1}{2}) = 180.7173447$ , both based on 2,036,000,000 TF-points. We have the *predicted* values  $G_{complex}(1) \approx 387.486102$  and  $G_{real}(1) \approx 114.6270015$ . (Searches using the “Plouffe’s Inverter” website <http://pi.lacim.uqam.ca/eng/> did not readily yield any underlying explanation of these values or a number of transformations of them.)

## V. FITTED INCOMPLETE BETA FUNCTIONS

Numerical computations (detailed in sec. IV above) — provided us with estimates of  $F_{complex}(\nu)$  and  $F_{real}(\nu)$  (though the sampling [quasi-Monte Carlo] procedure employed had been devised in terms of the variable  $\mu \equiv \sqrt{\nu}$  and counterpart functions  $f_{complex}(\mu)$  and  $f_{real}(\mu)$ ). We have been able to fit these results quite well (Fig. 4) using (concave) functions of the form (Fig. 3),

$$G_{real}(\nu) = \left(4 + \frac{1}{5\sqrt{2}}\right) B\left(\frac{1}{2}, \sqrt{3}\right)^8 B_\nu\left(\frac{1}{2}, \sqrt{3}\right) \quad (13)$$

and

$$G_{complex}(\nu) = \left(\frac{100000000}{2\sqrt[3]{2} + \frac{10^{3/4}}{3^{2/3}}}\right) B\left(\frac{2\sqrt{6}}{5}, \frac{3}{\sqrt{2}}\right)^{14} B_\nu\left(\frac{2\sqrt{6}}{5}, \frac{3}{\sqrt{2}}\right). \quad (14)$$

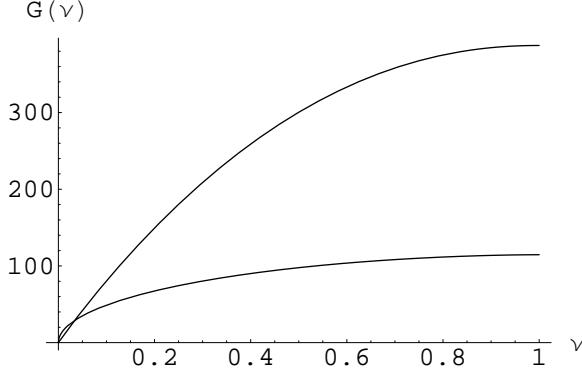


FIG. 3: The two fitted scaled incomplete beta functions  $G_{complex}(\nu)$  and the (lesser-valued at  $\nu = 1$ )  $G_{real}(\nu)$

(Let us note that  $\sqrt{3} \approx 1.73205$ ,  $\frac{2\sqrt{6}}{5} \approx 0.979796$  and  $\frac{3}{\sqrt{2}} \approx 2.12132$ .) Here  $B$  denotes the (complete) beta function, and  $B_\nu$  the *incomplete* beta function [44],

$$B_\nu(a, b) = \int_0^\nu w^{a-1}(1-w)^{b-1} dw. \quad (15)$$

(The beta function itself, that is  $B(a, b) \equiv B_1(a, b)$ , played an important instrumental role in the original formulation of string theory [45, p. 6]. For a more specific-still *incomplete* beta function role in string theory, pertaining to the symmetric group  $S_3$  and the modular group  $M(2)$ , see the review MR512916 of A. O. Barut in the MathSciNet database [<http://ams.rice.edu/mathscinet/>] of a [somewhat obscure] paper of M. Zăganescu [46].)

To obtain the two residual curves shown in Fig. 4 — upon which we draw our central conclusion that  $F_{real}(\nu)$  and  $F_{complex}(\nu)$  are well fitted by  $G_{real}(\nu)$  and  $G_{complex}(\nu)$ , respectively — we interpolated the Tezuka-Faure points, using third-order polynomials — and then reparameterized the resulting curve in terms of  $\nu$ .

### A. separable volume and hyperarea estimations

From the (exact) formulas of Życzkowski and Sommers [2] for the Hilbert-Schmidt volumes of the real and complex  $n \times n$  density matrices to the case  $n = 4$ , we know that the *total* volume of separable *and* nonseparable two-qubit systems is  $\frac{\pi^6}{851350500} \approx 1.12925 \cdot 10^{-6}$  in the 15-dimensional (complex) case and  $\frac{\pi^4}{60480} \approx 0.0016106$  in the 9-dimensional (real) case.

Also, from the results of Życzkowski and Sommers [2, eq. (6.5)], one can readily deduce that the ratio of boundary (14-dimensional) hyperarea to volume of the 15-dimensional

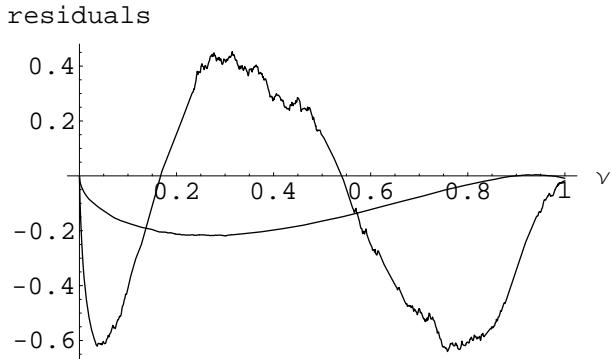


FIG. 4: Our numerical (interpolated) estimates (sec. IV) of  $F_{complex}(\nu)$  and  $F_{real}(\nu)$  minus the values predicted by  $G_{complex}(\nu)$  and  $G_{real}(\nu)$ . The more strongly fluctuating curve corresponds to the complex case. Note the greatly reduced  $y$ -axis scale *vis-à-vis* that of Fig. 3, this observation constituting the basis for our central assertion that the  $F(\nu)$ 's are well fitted by the  $G(\nu)$ 's.

convex set of  $4 \times 4$  density matrices is equal to  $30\sqrt{3}$ , and further [2, eq. (7.9)] that the corresponding (lesser) ratio for the 9-dimensional convex set of *real*  $4 \times 4$  density matrices is  $18\sqrt{3}$ . By the subsequent results of Szarek, Bengtsson and Życzkowski [10] — which were motivated by certain numerical analyses of Slater [8] — we know the analogous hyperarea-volume ratios for the 15- and 9-dimensional *separable* subsets must be simply *twice* as large (that is,  $60\sqrt{3}$  and  $36\sqrt{3}$ ).

Using the proposed incomplete beta function fits (13) and (14), we have attempted the evaluations of the two corresponding separable volumes ((8) and (9)), as well as separable (lower-dimensional) hyperareas, obtaining exact results in the complex case, but only numerical ones for the real scenario. We succeeded in the complex case, using integration-by-parts, first integrating  $Jac_{complex}(\nu)$ . (In the real case, an analogous initial integration of  $Jac_{real}(\nu)$  led to a much more complicated result, now involving various hypergeometric functions. So, the integration by parts was stymied there.) The exact result itself in the complex case (for which we thank M. Trott) was very lengthy (much too so to present here), but we could evaluate it to any given precision.

### 1. complex case

Using this *exact* formula, we were able to obtain  $V_{sep/complex} \approx 2.73827578 \cdot 10^{-7}$ , and again applying the Życzkowski-Sommers [2] and Szarek-Bengtsson-Życzkowski results [10],  $P_{sep/complex} \approx 0.24248582$  and  $H_{sep/complex} \approx 0.0000142285$ , all assuming the full applicability/validity of (14).

We had previously hypothesized that  $V_{sep/complex} = (5\sqrt{3})^{-7} \approx 2.73707 \cdot 10^{-7}$  [8, eq. (41)] and  $P_{sep/complex} = \frac{2^2 \cdot 3 \cdot 7^2 \cdot 11 \cdot 13 \sqrt{3}}{5^4 \pi^6} \approx 0.242379$  [8, eq. (43), but misprinted as  $5^3$  not  $5^4$  there]. The analysis in [8] was based on 400,000,000 quasi-Monte Carlo [Tezuka-Faure] points. (Those points were 15-dimensional in nature *vs.* the 12-dimensional ones used here.) Additionally, each point there was employed only *once* for the Peres-Horodecki separability test, while each point here is used in 2,000 such tests (with  $\mu$  ranging over  $[0,1]$ ). We had initially suspected that if we started checking the Peres-Horodecki criterion for successively larger values of  $\mu$ , holding the set of  $z_{ij}$ 's given by a Tezuka-Faure point *fixed*, then if we reached one value of  $\mu$  for which separability held, then *all* higher values of  $\mu$  (less than or equal to 1) would also yield separability. But this interestingly turned out not to be invariably the case. So, it appeared that we needed to check the criterion 2,000 times for every single 6-dimensional (real) or 12-dimensional (complex) TF-point.

### 2. real case

Since, as noted, exact integration-by-parts did not seem feasible in the real case, we chose to expand  $G_{real}(\nu)$  in a 75-term power series about  $\nu = 0$ , and performed *exact* integrations term-by-term. The overall result can be expressed as  $V_{sep/real} \approx 0.0007310253$ . Using the various results of Życzkowski and Sommers [2], and Szarek, Bengtsson and Życzkowski [10] detailed above, we then immediately have the estimates  $P_{sep/real} \approx 0.4538838$  for the separability *probability* of the real  $4 \times 4$  density matrices (markedly greater than in the complex case), and  $H_{sep/real} \approx 0.02279111$  for the hyperarea of the bounding 8-dimensional hypersurface.

## VI. CONCLUDING REMARKS

In this study, using the Bloore parameterization of density matrices ([19], sec. II), we have shown that incomplete beta functions (sec. V), or clearly quite close relatives to them, appear to play important roles in the calculation of the Hilbert-Schmidt separable volumes of the 9-dimensional real and 15-dimensional complex qubit-qubit pairs. However, there are still apparently systematic (sine-like) — although quite small — variations (Fig. 4) of the estimated function from the hypothesized one  $G_{\text{complex}}(\nu)$  in the complex case, so we suspect that we may have possibly not yet fully explained this scenario. So, to summarize, although we have developed here a rather compelling case for the relevance of the incomplete beta functions, our evidence for this is so far essentially empirical/numerical rather than theoretical.

The extension to qubit-*qutrit* pairs (and possibly higher-dimensional composite systems,  $n > 4$ ) of the *univariate*-function-strategy we have pursued above for the case of qubit-qubit pairs ( $n = 4$ ), seems problematical. In the  $n = 4$  case, the analysis is facilitated by the fact that it is sufficient that the *determinant* of the partial transpose of a density matrix be nonnegative for the Peres-Horodecki separability criterion to hold [36, Thm. 5] [47]. *More* requirements than this single one are needed in the qubit-qutrit scenario — even though the criterion of nonnegativity of the partial transpose is still *both* necessary and sufficient for  $6 \times 6$  density matrices. (In addition to the determinant, the leading minors and/or the individual eigenvalues of the partial transpose of the  $6 \times 6$  density matrix would need to be tested for nonnegativity, as well. Also the qubit-qutrit analogue of the ratio ( $\nu$ ) of diagonal entries, given by (6), would have to be defined, if even possible.)

In our earlier study [20], we had also employed the Bloore parameterization of the two-qubit (and qubit-qutrit) systems to study the Hilbert-Schmidt (HS) separability probabilities of specialized systems of *less* than full dimensionality. We also reported there an effort to determine a certain *three*-dimensional function (somewhat in contrast to the *one*-dimensional functions  $F_{\text{real}}(\nu)$  and  $F_{\text{complex}}(\nu)$  above, but for a rather similar purpose) over the simplex of eigenvalues that would facilitate the calculation of the 15-dimensional volume of the complex two-qubit systems in terms of (monotone) metrics — such as the Bures, Kubo-Mori, Wigner-Yanase, . . . — other than the (non-monotone [48]) Hilbert-Schmidt one considered here. (The Bloore parameterization [19] did not seem immediately useful in this monotone

metric context, since the *eigenvalues* of  $\rho$  are not explicitly expressed (cf. [49]). Therefore, we had recourse in [20] to the Euler-angle parameterization of density matrices of Tilma, Byrd and Sudarshan [23], in which the eigenvalues of  $\rho$  do, in fact, explicitly enter.)

So, it would seem to appear, initially at least, that the particular utility of the Bloore parameterization in reducing the dimensionality of the problem of computing the Hilbert-Schmidt separable volume of qubit-qubit pairs, of which we have taken advantage in this study, neither extends to higher-dimensional Hilbert-Schmidt volumes ( $n > 4$ ) nor to monotone metric volumes of even qubit-qubit pairs ( $n = 4$ ) themselves.

### Acknowledgments

I would like to express gratitude to the Kavli Institute for Theoretical Physics (KITP) for computational support in this research and to Michael Trott for his advice on computing the separable volumes (sec. V A).

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